



Training Deep Feedforwards Networks

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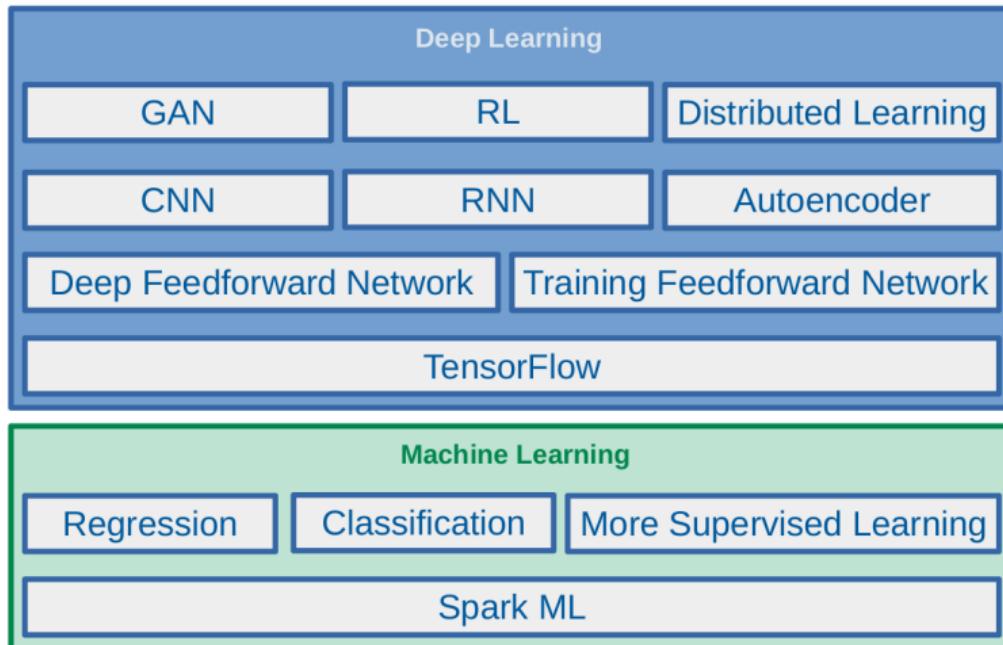


The Course Web Page

<https://id2223kth.github.io>

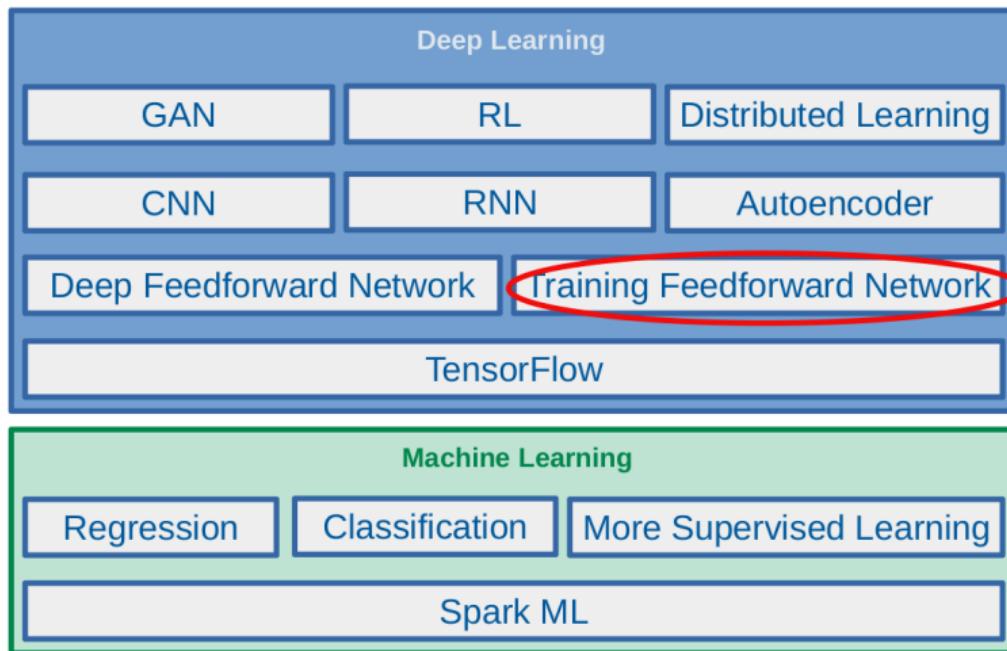


Where Are We?





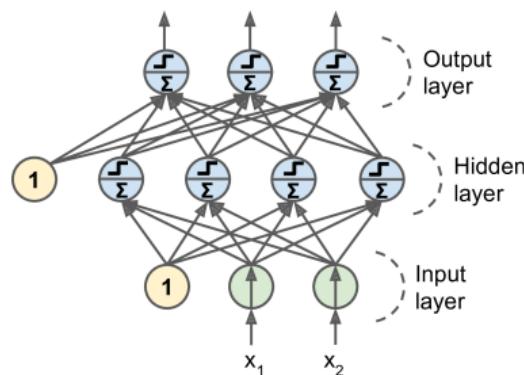
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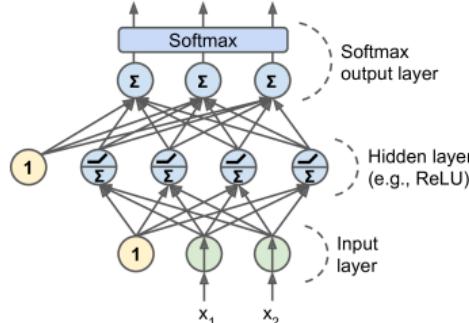
Feedforward Neural Network Architecture

- ▶ A **feedforward neural network** is composed of:

- One **input layer**
- One or more **hidden layers**
- One final **output layer**



Feedforward Network in TensorFlow



```
n_output = 3
n_hidden = 4
n_features = 2

model = keras.models.Sequential()
model.add(keras.layers.Dense(n_hidden, input_shape=(n_features,), activation="relu"))
model.add(keras.layers.Dense(n_output, activation="softmax"))

model.compile(loss="sparse_categorical_crossentropy", optimizer="sgd", metrics=["accuracy"])
model.fit(X_train, y_train, epochs=30)
```



Challenges of Training Feedforward Neural Networks

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Challenges of Training Feedforward Neural Networks

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- ▶ Overfitting: risk of overfitting a model with large number of parameters.
- ▶ Vanishing/exploding gradients: hard to train lower layers.
- ▶ Training speed: slow training with large networks.



Overfitting



High Degree of Freedom and Overfitting Problem

- ▶ With **large number of parameters**, a network has a **high degree of freedom**.
- ▶ It can **fit** a huge variety of **complex datasets**.



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- ▶ With **large number of parameters**, a network has a **high degree of freedom**.
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- ▶ This **flexibility** also means that it is **prone to overfitting on training set**.
- ▶ Let's **reduce** the degree of freedom a model.



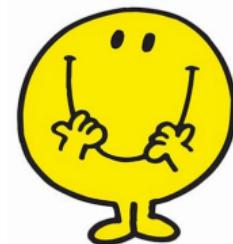
Avoiding Overfitting

- ▶ Early stopping
- ▶ ℓ_1 and ℓ_2 regularization
- ▶ Max-norm regularization
- ▶ Dropout
- ▶ Data augmentation



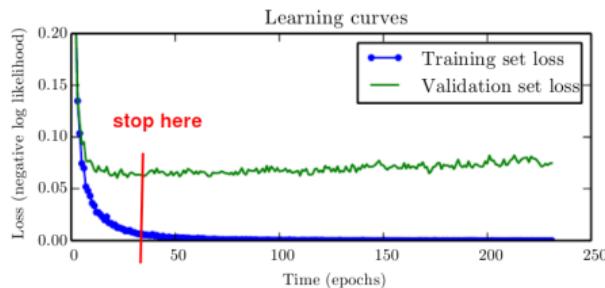
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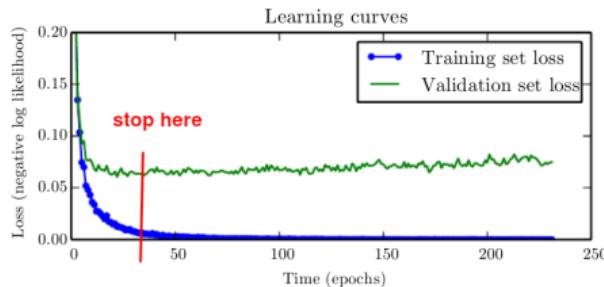
Early Stopping (1/2)

- ▶ As the **training steps go by**, its prediction error on the **training/validation set** naturally goes down.



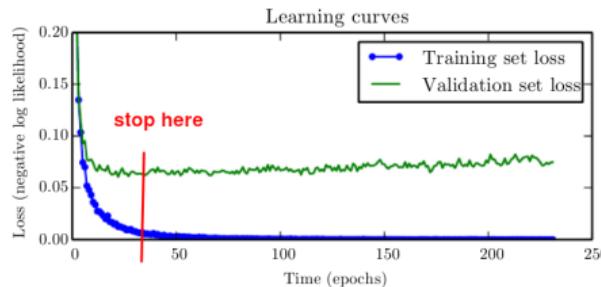
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- ▶ After a while the **validation error stops decreasing** and **starts to go back up**.
 - The model has started to **overfit the training data**.



Early Stopping (1/2)

- ▶ As the **training steps go by**, its prediction error on the **training/validation set** naturally **goes down**.
- ▶ After a while the **validation error stops decreasing** and **starts to go back up**.
 - The model has started to **overfit the training data**.
- ▶ In the **early stopping**, we **stop training** when the **validation error reaches a minimum**.





Early Stopping (2/2)

```
from tensorflow.keras.callbacks import EarlyStopping

model = tf.keras.models.Sequential(...)

model.compile(optimizer='sgd', loss='sparse_categorical_crossentropy', metrics=['accuracy'])

earlystop_callback = EarlyStopping(monitor='accuracy', min_delta=0.05, patience=1)

model.fit(x_train, y_train, epochs=500, callbacks=[earlystop_callback])
```

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ℓ_1 and ℓ_2 Regularization (1/3)

- ▶ Penalize **large values** of weights w_j .

$$\tilde{J}(\mathbf{w}) = J(\mathbf{w}) + \lambda R(\mathbf{w})$$

- ▶ Two questions:
 1. How should we define $R(\mathbf{w})$?
 2. How do we determine λ ?

/1 and /2 Regularization (2/3)

- **/1 regression:** $R(\mathbf{w}) = \lambda \sum_{i=1}^n |w_i|$ is added to the cost function.

$$\tilde{J}(\mathbf{w}) = J(\mathbf{w}) + \lambda \sum_{i=1}^n |w_i|$$

```
keras.layers.Dense(100, activation="relu", kernel_regularizer=keras.regularizers.l1(0.1))
```

/1 and /2 Regularization (3/3)

- **/2 regression:** $R(\mathbf{w}) = \lambda \sum_{i=1}^n w_i^2$ is added to the cost function.

$$\tilde{J}(\mathbf{w}) = J(\mathbf{w}) + \lambda \sum_{i=1}^n w_i^2$$

```
keras.layers.Dense(100, activation="relu", kernel_regularizer=keras.regularizers.l2(0.01))
```

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Max-Norm Regularization

- ▶ Max-norm regularization: constrains the weights w_j of the incoming connections for each neuron j .
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- ▶ After each training step, clip w_j as below, if $\|w_j\|_2 > r$:

$$w_j \leftarrow w_j \frac{r}{\|w_j\|_2}$$

- r is the max-norm hyperparameter
- $\|w_j\|_2 = (\sum_i w_{i,j}^2)^{\frac{1}{2}} = \sqrt{w_{1,j}^2 + w_{2,j}^2 + \dots + w_{n,j}^2}$



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```
keras.layers.Dense(100, activation="relu", kernel_constraint=keras.constraints.max_norm(1.))
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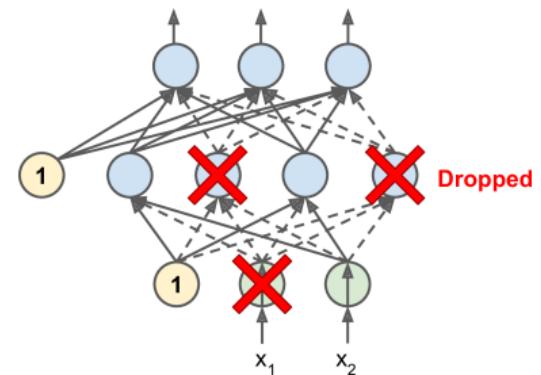
Dropout (1/4)

- ▶ Would a **company** perform better if its employees were told **to toss a coin** every morning to decide **whether or not to go to work**?



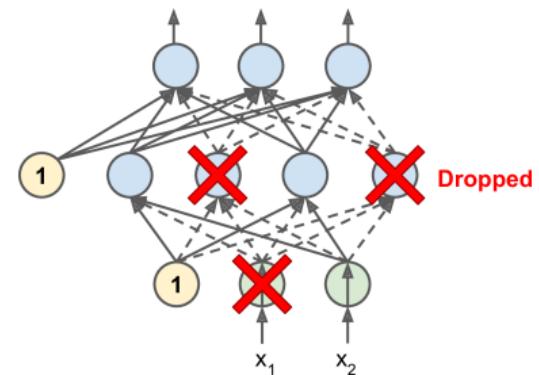
Dropout (2/4)

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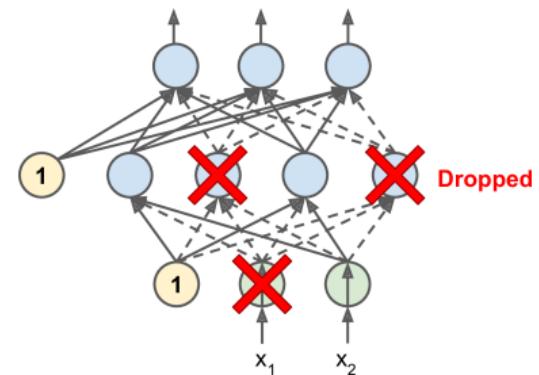
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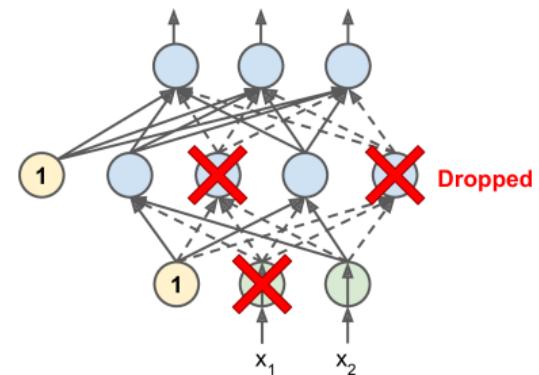
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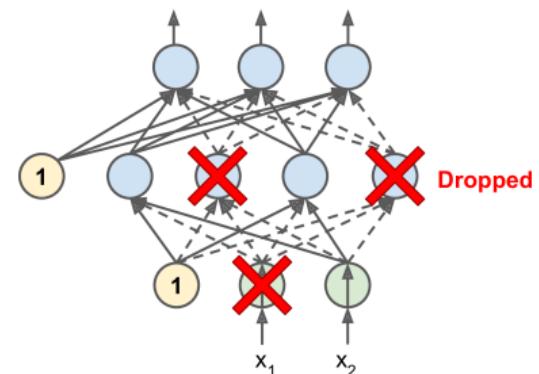
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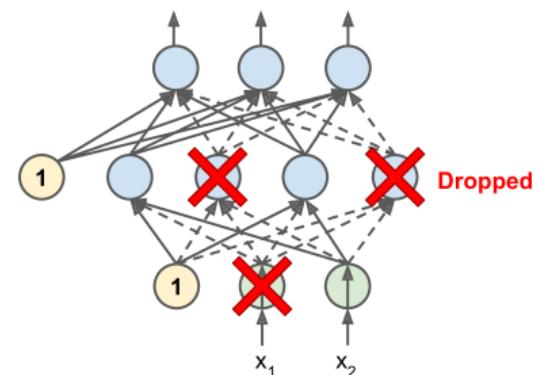
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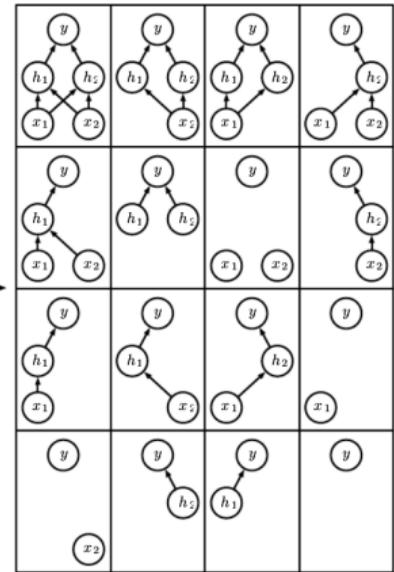
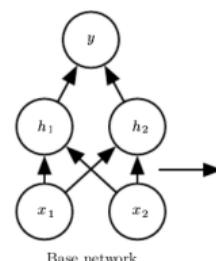
Dropout (2/4)

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 - The **hyperparameter p** is called the **dropout rate**.
 - A neuron will be **entirely ignored** during **this training step**.
 - It may be **active** during the **next step**.
 - Exclude the **output neurons**.
- ▶ After training, neurons don't get dropped anymore.



Dropout (3/4)

- ▶ Each neuron can be either **present or absent**.
- ▶ **2^N possible networks**, where **N** is the total number of **droppable neurons**.
 - **N = 4** in this figure.





Dropout (4/4)

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(128, activation="relu"),
    keras.layers.Dropout(rate=0.2),
    keras.layers.Dense(10, activation="softmax")
])
```

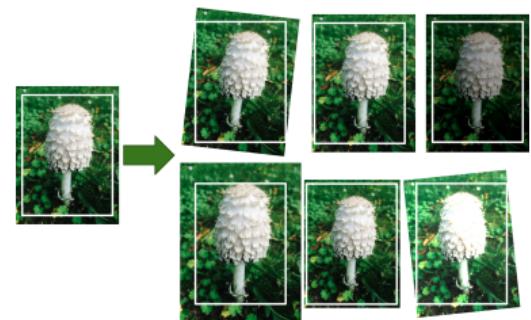
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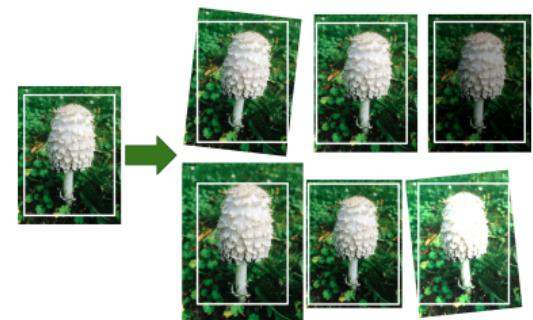
Data Augmentation

- ▶ One way to make a model **generalize better** is to **train it on more data**.
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Data Augmentation

- ▶ One way to make a model **generalize better** is to **train it on more data**.
- ▶ This will **reduce overfitting**.
- ▶ Create **fake data** and add it to the **training set**.
 - E.g., in an **image classification** we can slightly shift, rotate and resize an image.
 - Add the resulting pictures to the **training set**.



Vanishing/Exploding Gradients





Vanishing/Exploding Gradients Problem (1/4)

- ▶ The **backpropagation** goes from **output** to **input** layer, and propagates the **error gradient** on the way.

$$w^{(\text{next})} = w - \eta \frac{\partial J(w)}{\partial w}$$



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- ▶ Gradients often get smaller and smaller as the algorithm progresses down to the lower layers.
- ▶ As a result, the gradient descent update leaves the lower layer connection weights virtually unchanged.



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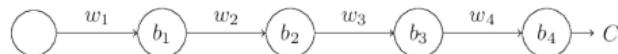
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- ▶ Gradients often get smaller and smaller as the algorithm progresses down to the lower layers.
- ▶ As a result, the gradient descent update leaves the lower layer connection weights virtually unchanged.
- ▶ This is called the vanishing gradients problem.

Vanishing/Exploding Gradients Problem (2/4)

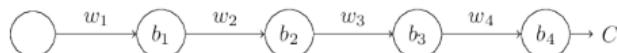
- ▶ Assume a network with just a single neuron in each layer.



- w_1, w_2, \dots are the weights
- b_1, b_2, \dots are the biases
- C is the cost function

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- ▶ The output a_j from the j th neuron is $\sigma(z_j)$.

- σ is the **sigmoid** activation function
- $z_j = w_j a_{j-1} + b_j$
- E.g., $a_4 = \sigma(z_4) = \text{sigmoid}(w_4 a_3 + b_4)$

Vanishing/Exploding Gradients Problem (3/4)

- ▶ Lets compute the **gradient** associated to the **first hidden neuron** ($\frac{\partial C}{\partial b_1}$).



$$\frac{\partial C}{\partial b_1} = \frac{\partial C}{\partial a_4} \times \frac{\partial a_4}{\partial z_4} \times \frac{\partial z_4}{\partial a_3} \times \frac{\partial a_3}{\partial z_3} \times \frac{\partial z_3}{\partial a_2} \times \frac{\partial a_2}{\partial z_2} \times \frac{\partial z_2}{\partial a_1} \times \frac{\partial a_1}{\partial z_1} \times \frac{\partial z_1}{\partial b_1}$$

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Vanishing/Exploding Gradients Problem (4/4)

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- ▶ Assume $w_3 \times \frac{\partial a_2}{\partial z_2} < \frac{1}{4}$ and $w_2 \times \frac{\partial a_1}{\partial z_1} < \frac{1}{4}$
 - The gradient $\frac{\partial C}{\partial b_1}$ be a factor of 16 (or more) smaller than $\frac{\partial C}{\partial b_3}$.
 - This is the essential origin of the vanishing gradient problem.

Overcoming the Vanishing Gradient

- ▶ Parameter initialization strategies
- ▶ Nonsaturating activation function
- ▶ Batch normalization
- ▶ Gradient clipping



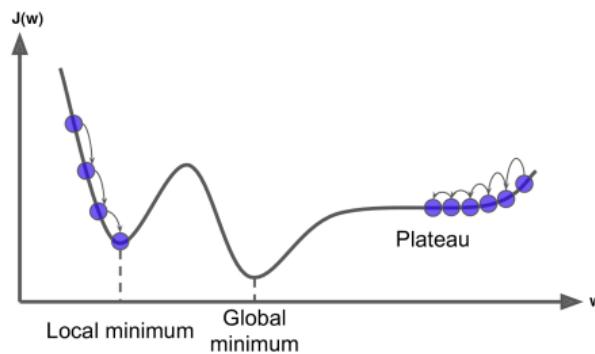
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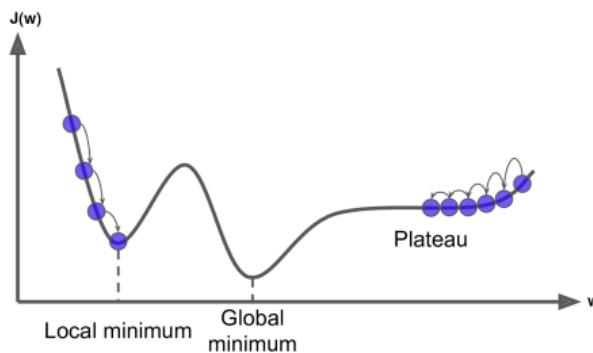
Parameter Initialization Strategies (1/4)

- The non-linearity of a neural network causes the cost functions to become non-convex.



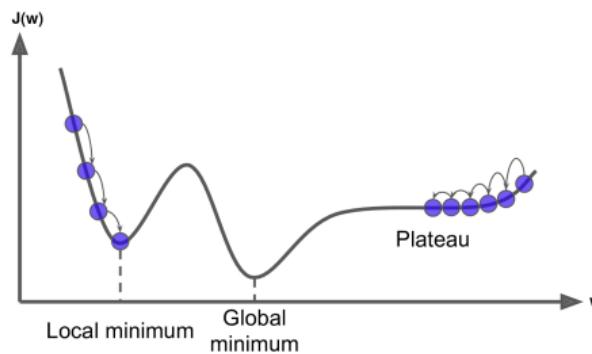
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Parameter Initialization Strategies (1/4)

- ▶ The **non-linearity** of a neural network causes the **cost functions** to become **non-convex**.
- ▶ The stochastic gradient descent on **non-convex cost functions** performs is **sensitive** to the values of the **initial parameters**.
- ▶ Designing initialization strategies is a **difficult task**.





Parameter Initialization Strategies (2/4)

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- ▶ **Two hidden units** with the **same activation function** connected to the **same inputs**, must have **different** initial parameters.
 - The goal of having each unit **compute a different function**.
- ▶ It motivates **random initialization** of the parameters.
 - Typically, we set the **biases** to **constants**, and initialize only the **weights randomly**.



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 - The **gradients** to have **equal variance before and after** flowing through a layer in the reverse direction.
- ▶ It is not possible to guarantee both unless each layer has an **equal number of inputs and neurons**.
- ▶ Based on the **Xavier initialization**, the weights are **initialized** using **normal distribution** with **mean 0** and the following **standard deviation**.



Parameter Initialization Strategies (4/4)

- ▶ fan_{in} and fan_{out} are the **number of inputs and neurons** for the layer whose weights are being initialized.
- ▶ $\text{fan}_{\text{avg}} = \frac{2}{\text{fan}_{\text{in}} + \text{fan}_{\text{out}}}$



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```
keras.layers.Dense(10, activation="relu", kernel_initializer="he_normal")
```

Overcoming the Vanishing Gradient

- ▶ Parameter initialization strategies
- ▶ Nonsaturating activation function
- ▶ Batch normalization
- ▶ Gradient clipping

by Roger Hargreaves





Nonsaturating Activation Functions (1/4)

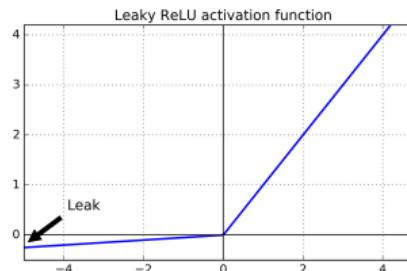
- ▶ $\text{ReLU}(z) = \max(0, z)$
- ▶ The **dying ReLUs** problem.

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- ▶ $\text{ReLU}(z) = \max(0, z)$
- ▶ The **dying ReLUs** problem.
 - During **training**, some neurons **stop outputting anything other than 0**.
 - E.g., when the **weighted sum of the neuron's inputs is negative**, it starts outputting 0.
- ▶ Use **leaky ReLU** instead: $\text{LeakyReLU}_\alpha(z) = \max(\alpha z, z)$.
 - α is the **slope** of the function for $z < 0$.





Nonsaturating Activation Functions (2/4)

► Randomized Leaky ReLU (RReLU)

- α is picked **randomly** during training, and it is **fixed** during testing.



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 - Learn α **during training** (instead of being a hyperparameter).

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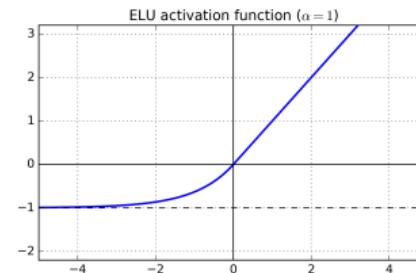
- α is picked **randomly** during training, and it is **fixed** during testing.

► Parametric Leaky ReLU (PReLU)

- Learn α **during training** (instead of being a hyperparameter).

► Exponential Linear Unit (ELU)

$$\text{ELU}_\alpha(z) = \begin{cases} \alpha(\exp(z) - 1) & \text{if } z < 0 \\ z & \text{if } z \geq 0 \end{cases}$$



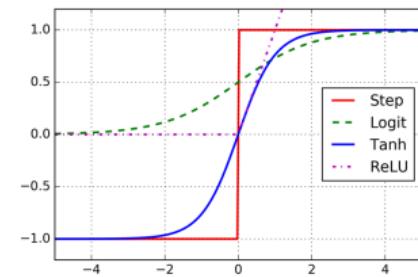
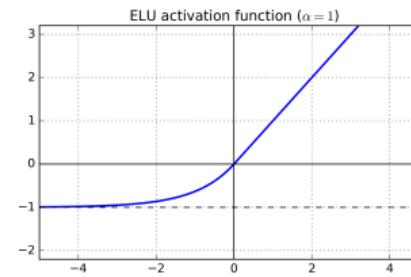
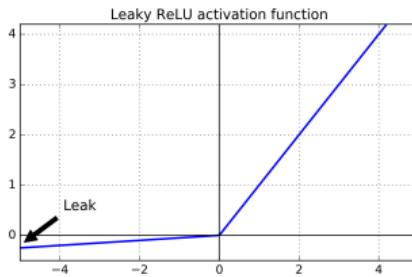


Nonsaturating Activation Functions (3/4)

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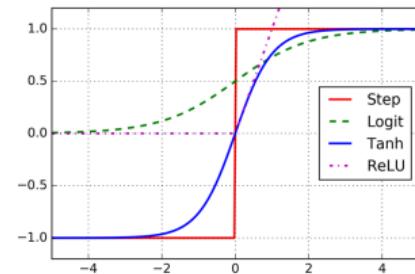
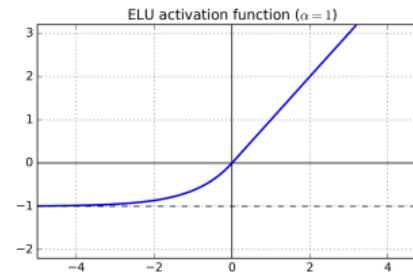
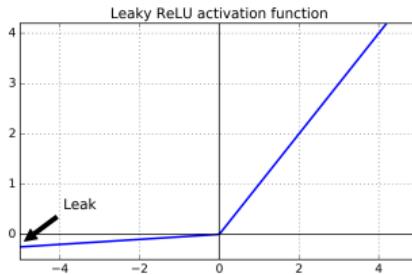
Nonsaturating Activation Functions (3/4)

- ▶ Which activation function should we use?
- ▶ In general logistic < tanh < ReLU < leaky ReLU (and its variants) < ELU



Nonsaturating Activation Functions (3/4)

- ▶ Which activation function should we use?
- ▶ In general logistic < tanh < ReLU < leaky ReLU (and its variants) < ELU
- ▶ If you care about runtime performance, then leaky ReLUs works better than ELUs.





Nonsaturating Activation Functions (4/4)

```
# elu
keras.layers.Dense(10, activation="elu")
```



Nonsaturating Activation Functions (4/4)

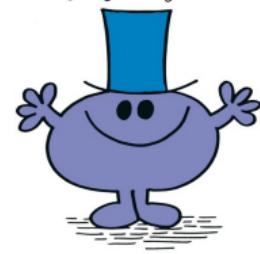
```
# elu
keras.layers.Dense(10, activation="elu")
```

```
# leaky relu
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(128, kernel_initializer="he_normal"),
    keras.layers.LeakyReLU(),
    keras.layers.Dense(10, activation="softmax")
])
```

Overcoming the Vanishing Gradient

- ▶ Parameter initialization strategies
- ▶ Nonsaturating activation function
- ▶ **Batch normalization**
- ▶ Gradient clipping

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Batch Normalization (1/4)

- ▶ The gradient tells how to update each parameter, under the assumption that the other layers do not change.



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 - In practice, we update all of the layers simultaneously.
 - However, unexpected results can happen.
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 - It is a technique to address the problem that the distribution of each layer's inputs changes during training, as the parameters of the previous layers change.



Batch Normalization (1/4)

- ▶ The gradient tells how to **update each parameter**, under the assumption that **the other layers do not change**.
 - In practice, we update all of the layers **simultaneously**.
 - However, **unexpected results can happen**.
- ▶ **Batch normalization** makes the **learning of layers** in the network more **independent of each other**.
 - It is a technique to address the problem that the **distribution of each layer's inputs** changes **during training**, as the parameters of the previous layers change.
- ▶ The technique consists of **adding an operation** in the model just **before the activation function** of each layer.



Batch Normalization (2/4)

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 - Estimates the inputs' mean and standard deviation of the current mini-batch.

$$\mu_B = \frac{1}{m_B} \sum_{i=1}^{m_B} x^{(i)}$$

$$\sigma_B^2 = \frac{1}{m_B} \sum_{i=1}^{m_B} (x^{(i)} - \mu_B)^2$$

- ▶ μ_B : the empirical mean, evaluated over the whole mini-batch B .
- ▶ σ_B^2 : the empirical standard deviation, also evaluated over the whole mini-batch.
- ▶ m_B : the number of instances in the mini-batch.



Batch Normalization (3/4)

$$\hat{x}^{(i)} = \frac{x^{(i)} - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$
$$z^{(i)} = \gamma \hat{x}^{(i)} + \beta$$

- ▶ $\hat{x}^{(i)}$: the zero-centered and normalized input.
- ▶ γ : the scaling parameter for the layer.
- ▶ β : the shifting parameter (offset) for the layer.
- ▶ ϵ : a tiny number to avoid division by zero.
- ▶ $z^{(i)}$: the output of the BN operation, which is a scaled and shifted version of the inputs.



Batch Normalization (4/4)

```
model = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.BatchNormalization(),
    keras.layers.Dense(128, activation="relu"),
    keras.layers.BatchNormalization(),
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```

Overcoming the Vanishing Gradient

- ▶ Parameter initialization strategies
- ▶ Nonsaturating activation function
- ▶ Batch normalization
- ▶ **Gradient clipping**

Roger Hargreaves





Gradient Clipping

- ▶ **Gradient clipping:** clip the gradients during **backpropagation** so that they **never exceed some threshold**.

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optimizer = keras.optimizers.SGD(clipvalue=1.0)
model.compile(loss="mse", optimizer=optimizer)
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- ▶ `clipvalue=1.0`: $[0.9, 100.0] \Rightarrow [0.9, 1.0]$



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- ▶ **clipvalue=1.0**: $[0.9, 100.0] \Rightarrow [0.9, 1.0]$
- ▶ **clipnorm=1.0**: $[0.9, 100.0] \Rightarrow [0.00899964, 0.9999595]$

Training Speed

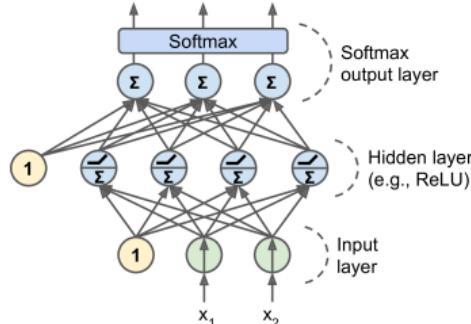




Regular Gradient Descent Optimization (1/2)

- ▶ Gradient descent optimization algorithm
- ▶ It updates the weights $w_i^{(\text{next})} = w - \eta \frac{\partial J(w)}{\partial w_i}$
- ▶ Better optimization algorithms to improve the training speed

Regular Gradient Descent Optimization (2/2)



```
n_output = 3
n_hidden = 4
n_features = 2

model = keras.models.Sequential()
model.add(keras.layers.Dense(n_hidden, input_shape=(n_features,), activation="relu"))
model.add(keras.layers.Dense(n_output, activation="softmax"))

model.compile(loss="sparse_categorical_crossentropy", optimizer="sgd", metrics=["accuracy"])
model.fit(X_train, y_train, epochs=30)
```

Optimization Algorithms

- ▶ Momentum
- ▶ Nesterov momentum
- ▶ AdaGrad
- ▶ RMSProp
- ▶ Adam Optimization





Optimization Algorithms

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Momentum (1/3)

- ▶ Momentum is a concept from physics: an object in motion will have a tendency to keep moving.
- ▶ It measures the resistance to change in motion.
 - The higher momentum an object has, the harder it is to stop it.



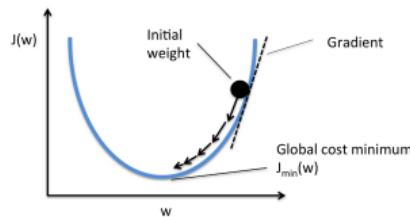


Momentum (2/3)

- ▶ This is the very simple idea behind **momentum optimization**.

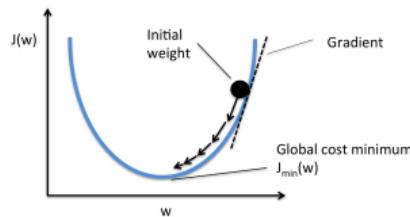
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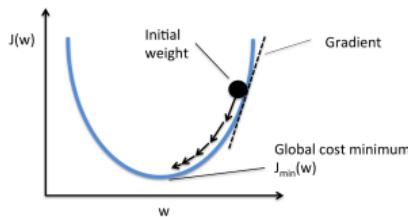
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- ▶ We can thus use the concept of momentum to give the update process a **tendency to keep moving** in the same direction.
- ▶ It can help to **escape from bad local minima pits**.





Momentum (3/3)

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- ▶ At each iteration, it adds the **local gradient** to the momentum vector **m**.

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```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

Optimization Algorithms

- ▶ Momentum
- ▶ Nesterov momentum
- ▶ AdaGrad
- ▶ RMSProp
- ▶ Adam optimization

By Roger Hargreaves



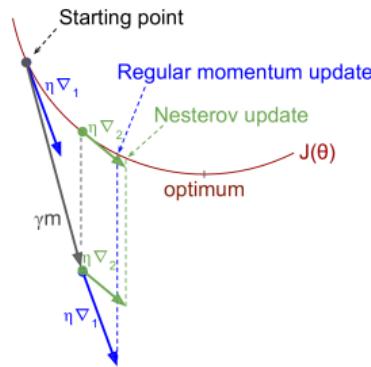


Nesterov Momentum (1/2)

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- ▶ Faster than vanilla Momentum optimization.

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- ▶ Nesterov Momentum is a small variant to Momentum optimization.
- ▶ Faster than vanilla Momentum optimization.
- ▶ ∇_1 represents the gradient of the cost function measured at the starting point w , and ∇_2 represents the gradient at the point located at $w + \beta m$.





Nesterov Momentum (2/2)

- ▶ Measure the gradient of the cost function slightly ahead in the direction of the momentum (not at the local position).

$$w_i^{(\text{next})} = w_i - (-\beta m_i + \eta \frac{\partial J(w + \beta m)}{\partial w_i})$$



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```
optimizer = keras.optimizers.SGD(lr=0.001, momentum=0.9, nesterov=True)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```



Optimization Algorithms

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- ▶ Nesterov momentum
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AdaGrad (1/2)

- ▶ AdaGrad keeps track of a learning rate for each parameter.
- ▶ Adapts the learning rate over time (adaptive learning rate).
- ▶ Decays the learning rate faster for steep dimensions than for dimensions with gentler slopes.



AdaGrad (2/2)

- ▶ For each feature w_i , we do the following steps:

$$s_i = s_i + \left(\frac{\partial J(\mathbf{w})}{\partial w_i} \right)^2$$

$$w_i^{(\text{next})} = w_i - \frac{\eta}{\sqrt{s_i + \epsilon}} \frac{\partial J(\mathbf{w})}{\partial w_i}$$



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```
optimizer = keras.optimizers.Adagrad(lr=0.001)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```

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- ▶ Nesterov momentum
- ▶ AdaGrad
- ▶ RMSProp
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RMSProp (1/2)

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- ▶ The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum.



RMSProp (1/2)

- ▶ AdaGrad often stops too early when training neural networks.
- ▶ The learning rate gets scaled down so much that the algorithm ends up stopping entirely before reaching the global optimum.
- ▶ The RMSProp fixed the AdaGrad problem.
- ▶ It is like the AdaGrad problem, but accumulates only the gradients from the most recent iterations (not from the beginning of training).



RMSProp (2/2)

- ▶ For each feature w_i , we do the following steps:

$$\begin{aligned}s_i &= \beta s_i + (1 - \beta) \left(\frac{\partial J(w)}{\partial w_i} \right)^2 \\w_i^{(\text{next})} &= w_i - \frac{\eta}{\sqrt{s_i + \epsilon}} \frac{\partial J(w)}{\partial w_i}\end{aligned}$$



RMSProp (2/2)

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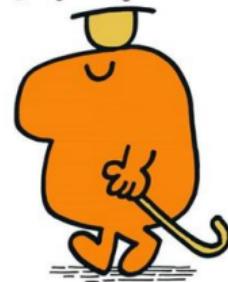
```
optimizer = keras.optimizers.RMSprop(lr=0.001, rho=0.9)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```



Optimization Algorithms

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Adam Optimization (1/3)

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- ▶ Like Momentum optimization, it keeps track of an exponentially decaying average of past gradients.
- ▶ Like RMSProp, it keeps track of an exponentially decaying average of past squared gradients.



Adam Optimization (2/3)

$$1. \quad \mathbf{m}^{(\text{next})} = \beta_1 \mathbf{m} + (1 - \beta_1) \nabla_{\mathbf{w}} J(\mathbf{w})$$

$$2. \quad \mathbf{s}^{(\text{next})} = \beta_2 \mathbf{s} + (1 - \beta_2) \nabla_{\mathbf{w}} J(\mathbf{w}) \otimes \nabla_{\mathbf{w}} J(\mathbf{w})$$

$$3. \quad \mathbf{m}^{(\text{next})} = \frac{\mathbf{m}}{1 - \beta_1^T}$$

$$4. \quad \mathbf{s}^{(\text{next})} = \frac{\mathbf{s}}{1 - \beta_2^T}$$

$$5. \quad \mathbf{w}^{(\text{next})} = \mathbf{w} - \eta \mathbf{m} \oslash \sqrt{\mathbf{s} + \epsilon}$$

- ▶ \otimes and \oslash represents the represents the element-wise multiplication and division.
- ▶ Steps 1, 2, and 5: similar to both Momentum optimization and RMSProp.
- ▶ Steps 3 and 4: since \mathbf{m} and \mathbf{s} are initialized at 0, they will be biased toward 0 at the beginning of training, so these two steps will help boost \mathbf{m} and \mathbf{s} at the beginning of training.



Adam Optimization (3/3)

```
optimizer = keras.optimizers.Adam(lr=0.001, beta_1=0.9, beta_2=0.999)
model.compile(loss="sparse_categorical_crossentropy", optimizer=optimizer, metrics=["accuracy"])
```



Summary

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- ▶ Overfitting
 - Early stopping, ℓ_1 and ℓ_2 regularization, max-norm regularization
 - Dropout, data augmentation
- ▶ Vanishing gradient
 - Parameter initialization, nonsaturating activation functions
 - Batch normalization, gradient clipping
- ▶ Training speed
 - Momentum, nesterov momentum, AdaGrad
 - RMSProp, Adam optimization





Reference

- ▶ Ian Goodfellow et al., Deep Learning (Ch. 7, 8)
- ▶ Aurélien Géron, Hands-On Machine Learning (Ch. 11)



Questions?